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Synthesis and Molecular Structure of
closo-3-(η^6 -C₆H₆)-3,1,2-FeC₂B₉H₁₁

by

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Synthesis and molecular structure of *closo*-3-(η^6 -C₆H₆)-3,1,2-FeC₂B₉H₁₁ *

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Abstract

The mixed-sandwich complex, *closo*-3-(η^6 -C₆H₆)-3,1,2-FeC₂B₉H₁₁ (**2**), has been prepared in high yield by the photolysis of *closo*-3,3,3-(CO)₃-3,1,2-FeC₂B₉H₁₁ (**1**) in benzene. The molecular structure of **2** has been determined by an X-ray diffraction study. Compound **2** crystallized in the orthorhombic space group *Pmcn* (standard setting *Pnma*) with *a* 7.693(1) Å, *b* 9.001(2) Å, *c* 18.420(3) Å, *V* 1276 Å³, and *Z* = 4 (8 half molecules related by a mirror plane at *x* = 1/4). The structure was solved by heavy atom methods to a final discrepancy index of *R* = 0.053, *R*_w = 0.067 for 861 independent reflections.

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